Doping dependence of density response and bond-stretching phonons in cuprates

Peter Horsch * Giniyat Khaliullin

Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

Abstract

We explain the anomalous doping dependence of zone boundary $(\pi, 0)$ and (π, π) bond-stretching phonons in $La_{2-\delta}Sr_{\delta}CuO_4$ in the range $0 < \delta < 0.35$. Our calculations are based on a theory for the density response of doped Mott-Hubbard insulators.

Key words:
High temperature superconductors, LaSrCuO, Density response of doped Mott-Hubbard insulator, bond-stretching phonons

The relevance of electron-phonon interaction for high-T_c superconductivity has been controversially discussed over the years. Certainly a clear signature of the interplay of charge carriers and phonons is the strong dependence of breathing and bond-stretching phonon modes as function of doping as evidenced in neutron scattering data. This was first oberved in LaSrCuO and YBCO [1,2], yet appears meanwhile as a generic feature of all high-T_c superconductors.

The theoretical study of phonon renormalization in strongly correlated high-T_c superconductors requires a calculation of the density response for a doped Mott-Hubbard insulator (MHI). Such a theory has been developed for the t-J model based on a description of correlated electrons in the framework of the slave boson approach [3], as well as within the complementary slave fermion method [4], with results in favorable agreement with exact diagonalization studies [5].

In this contribution we report the doping dependence for $La_{2-\delta}Sr_{\delta}CuO_4$ in the range $0 < \delta < 0.35$ of the zone-boundary (π, π) breathing phonon and of the highly anomalous $(\pi, 0)$ bond-stretching mode, i.e., calculated by means of the slave boson approach [3].

* Corresponding Author: Max-Planck-Institut FKF, D-70569 Stuttgart, Germany. Phone: +49 711 689-1550 Fax: +48 711 689-1702, Email: P.Horsch@fkf.mpg.de

The phonon data presented include theoretical results for optimal doping, $\delta = 0.15$, published earlier [6].

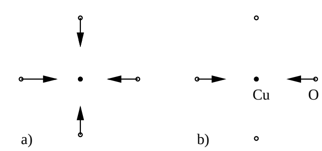

Fig. 1. Displacements of O ions (a) for $\mathbf{q} = (\pi, \pi)$ and (b) for the $(\pi, 0)$ half-breathing mode.

The phonon modes under discussion couple directly to the density of holes $n_i^h = h_i^+ h_i$ since the associated O-ion displacements lead to a modulation of the Zhang-Rice singlet energy. This is also the reason why the renormalization of these phonons can be treated in the framework of the t-J model. The change of the Zhang-Rice energy $E_{ZR} = 8t_{pd}^2/\Delta\epsilon$ with respect to the oxygen displacements u_α^i, $\alpha = x, y$, of the four O-neighbors at $R_i + \delta_\alpha^O$ around the Cu-hole at R_i yields the linear electron-phonon coupling [6]

$$H_{e-ph} = g \sum_i (u_x^i - u_{-x}^i + u_y^i - u_{-y}^i) h_i^+ h_i. \quad (1)$$

We assume that the resonance integral obeys the Harrison relation $t_{pd} \propto r_0^{-7/2}$, where r_0 is the Cu-O distance, and obtain $g = 7E_{ZR}/4r_0$, i.e., $g \approx 2\mathrm{eV/Å}$. The lattice part of the Hamiltonian is determined by the force

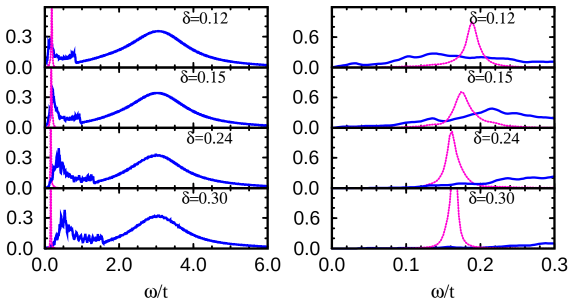

Fig. 2. Dynamic charge structure factor $N(\mathbf{q},\omega)$ (*normalized by the density of holes* δ) at momentum $\mathbf{q}=(\pi,0)$ for different doping concentrations δ. (a) On the large energy scale revealing the scaling of the edge of the spinon particle hole continuum $\sim 4(\kappa J+\delta t)$ and of the polaron peak $\sim(\kappa J+\delta t)$. (b) $N(\mathbf{q},\omega)$ at low energy and doping dependence of the spectral function of the $\mathbf{q}=(\pi,0)$ bond stretching phonon.

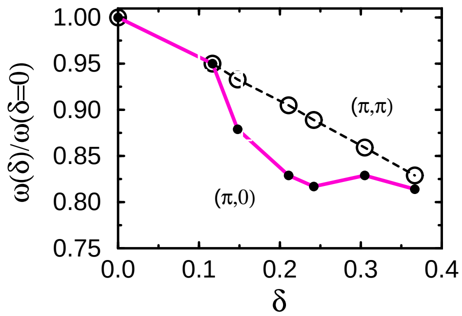

Fig. 3. Predicted doping dependence on the basis of the t-J model for (π,π) breathing and $(\pi,0)$ bond-stretching phonon energies in $La_{2-\delta}Sr_\delta CuO_4$. Parameters as for Fig.2: $t=0.4$ eV, $J/t=0.3$, and dimensionless electron phonon coupling constant $\xi=g^2/ztK\simeq 0.06$.

constant $K\approx 25\mathrm{eV}/\text{Å}^2$ for the longitudinal O-motion. Due to the structure of H_{e-ph} the bond stretching modes couple directly to the density response function $\chi(\mathbf{q},\omega)$. We have studied the renormalization of the phonon Green's function

$$D^{ph}_{\mathbf{q},\omega}=\frac{\omega_{\mathbf{q},0}}{\omega^2-\omega^2_{\mathbf{q},0}(1-\alpha_{\mathbf{q}}\chi(\mathbf{q},\omega))}, \tag{2}$$

where $\omega_{\mathbf{q},0}$ is the bare phonon frequency, i.e. measured in the undoped parent compound ($\omega_{\mathbf{q},0}\sim 80$ and 90 meV for $(\pi,0)$ and (π,π), respectively [1]). The coupling function $\alpha_{\mathbf{q}}=\frac{4g^2}{K}(\sin^2 q_x/2+\sin^2 q_y/2)$ vanishes at the Γ point and becomes maximal at the zone edges. Based on the parameters of the pd-model we estimate for the dimensionless coupling constant $\xi=g^2/ztK\sim 0.07-0.12$.

The central quantity controlling the phonon propagator, Eq.(2), is of course the density response function $\chi(\mathbf{q},\omega)=\langle\delta n^h\delta n^h\rangle_{\mathbf{q}\omega}$ of the doped Mott-Hubbard insulator, whose momentum and frequency dependence was studied in Ref.[3]. Figure 2(a) shows the doping dependence of the associated density fluctuation spectrum $N(\mathbf{q},\omega)=\frac{1}{\pi}\chi''(\mathbf{q},\omega)/\delta$ for $\mathbf{q}=(\pi,0)$. At $\mathbf{q}=(\pi,0)$ the main structure of $N(\mathbf{q},\omega)$ lies at high energy $\sim 3t$ and is strongly broadened due to the scattering of holes by spin excitations. The underlying polaronic mechanism leads at the same time to a peak in $N(\mathbf{q},\omega)$ at low energy $\sim(\kappa J+\delta t)$ with $\kappa\sim 0.3$, which can be attributed to the coherent motion of the polarons, i.e., holes dressed by spin excitations moving coherently on the energy scale dictated by the spin degrees of freedom. This polaron peak, whose energy scales with δ, is the origin of the anomalous behavior of the $(\pi,0)$ bond-stretching phonon. Interestingly this polaron structure is absent near (π,π)[5,3], hence no anomalous behavior is expected for the breathing phonon. The origin of the anomalous behavior of the density response of the doped MHI near $(\pi,0)$ can be traced back to a strong $(\pi,0)\leftrightarrow(0,\pi)$ scattering mediated by spin-excitations with momentum transfer close to (π,π). An additional feature seen in Fig. 2(a) is the spinon particle-hole continuum which at $(\pi,0)$ extends up to $\sim 4(\kappa J+\delta t)$.

As $\chi(\mathbf{q},\omega)$ is proportional to the hole density, phonons are renormalized basically linearly with δ, yet due to the polaron structure at low energy along the $(\pi,0)$ direction, the $(\pi,0)$ phonon reveals an anomalous energy shift and damping. The strong doping dependence of this effect, shown in Fig.2(b) and Fig.3, is due to the shift $\propto(\kappa J+\delta t)$ of the polaron peak position in $N(\mathbf{q},\omega)$ and its crossing of the bond-stretching phonon energy. Our results imply in particular that the large damping of the $(\pi,0)$ optical phonon near optimal doping disappears at larger doping concentrations, where the two phonon modes $(\pi,0)$ and (π,π) behave similar.

In conclusion, the anomalous renormalization and damping of bond stretching phonons is a manifestation of the strongly correlated motion of holes in cuprates, thus the study of these phonons provides a subtle test of the low-energy density response in cuprates at finite momentum transfer.

References

[1] L. Pintschovius and W. Reichardt, in *Physical Properties of High Temperature Superconductors IV*, ed. by D. Ginsberg (World Scientific, Singapore, 1994), p. 295.

[2] L. Pintschovius and M. Braden, Phys. Rev. B 60, R15039 (1999).

[3] G. Khaliullin and P. Horsch, Phys. Rev. B 54 (1996) R9600.

[4] P. Horsch, G. Khaliullin, and V. Oudovenko, Physica C, 341-348, 117 (2000).

[5] T. Tohyama, P. Horsch and S. Maekawa, Phys. Rev. Lett. 74 (1995) 980.

[6] G. Khaliullin and P. Horsch, Physica C 282-287 (1997) 1751.